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**Effects of including the adjoint sea ice rheology on estimating Arctic ocean-sea ice state**

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**Abstract.** The adjoint assimilation method has been applied to coupled ocean and sea ice models for sensitivity studies and Arctic state estimations. However, the accuracy of the adjoint model is degraded by simplifications of the adjoint of the sea ice model, especially the adjoint sea ice rheologies. As part of ongoing developments in coupled ocean and sea ice estimation systems, we incorporate and approximate the adjoint of viscous-plastic sea ice dynamics (adjoint-VP) and compare it with the adjoint of a free drift sea ice dynamic (adjoint-FD) through assimilation experiments. Using the adjoint-VP results in a further cost reduction of 7.9% in comparison to adjoint-FD, with noticeable improvements in the ocean temperature over the open water and the intermediate layers of the Arctic Ocean. Adjoint-VP more efficiently adjusts the uncertain model inputs more efficiently than does adjoint-FD by involving different sea ice retreat processes. For instance, adjoint-FD melts the sea ice up to 1.0 m in the marginal seas from May to June by over-adjusting air temperature (>8 °C); adjoint-VP reproduces the sea ice retreat with smaller adjustments to the atmospheric state within their prior uncertainty range. These developments of the adjoint model here lay the foundation for further improving Arctic Ocean and sea ice estimationS by comprehensively adjusting the initial conditions, atmospheric forcings, and uncertain parameters of the model.

## 28 **1 Introduction**

29 The Arctic Ocean has experienced drastic changes, including rapidly declining sea ice (Comiso et al., 2008;  
30 Kwok, 2018), increased inventory of freshwater in the western Arctic (Proshutinsky et al., 2019), enhanced warm  
31 inflows from the Pacific Ocean (Woodgate et al., 2012) and the Atlantic Ocean (Polyakov et al., 2017; Quadfasel et  
32 al., 1991), and increased ocean primary productivity (AMAP, 2021), and has been migrating to a new state over the  
33 past decades. These changes potentially impact the climate and weather of the Northern Hemisphere (Ma et al., 2022;  
34 Overland et al., 2021).

35 In recent years, progress has been made in satellite techniques (e.g., Kaleschke et al., 2001; Spreen et al., 2008),  
36 in-situ observations (e.g., Toole et al., 2016; Morison et al., 2007; Polyakov et al., 2017; Proshutinsky et al., 2009;  
37 Schauer et al., 2008), and coupled ocean and sea ice models. However, the lack of extensive Arctic observations,  
38 especially direct observations of the state variables and fluxes through the water column, and the deficiencies in the  
39 coupled ocean and sea-ice model still obscure our understanding of the Arctic sea ice changes and extremes. Accurate  
40 predictions of sea ice are therefore limited (e.g., Yang et al., 2020).

41 To fill the gaps, research groups have applied data assimilation techniques to ingest available observations into  
42 coupled ocean and sea ice models. The resulting reanalyses are assumed to have higher accuracy since as the  
43 development of models and data assimilation methods progress and the observation numbers increase. Most of Arctic  
44 coupled ocean and sea ice data assimilation and operational forecasting systems use statistical methods such as optimal  
45 interpolation (e.g., Lindsay and Zhang, 2006) and ensemble Kalman filters (e.g., Mu et al., 2018; Sakov et al., 2012).  
46 The advantage of these statistical methods is that they ensure a local fit to available observations (within prior  
47 uncertainties of both model and observations). However, away from the observations and for the unobserved variables,  
48 these methods rely on the inaccurate spatial covariance of model states for interpolation. In addition, these algorithms  
49 can introduce artificial sink/source terms to the numerical models, violating the model physics.

50 Over recent decades, an adjoint method with a large assimilation window (years to decades) has been developed in  
51 the framework of Estimating the Circulation and Climate of the Ocean (ECCO, Heimbach et al., 2019; Stammer et al.,  
52 2002; Wunsch and Heimbach, 2007) to create dynamically consistent ocean reanalyses. This method iteratively  
53 minimises a cost function that measures the model-data “distance” by adjusting model uncertain inputs (control  
54 variables). The use of an adjoint model (adjoint of the tangent linear approximation of the nonlinear model) as a  
55 spatiotemporal interpolator distinguishes this method from the statistical methods. In addition, the adjoint method  
56 adjusts all uncertain inputs, including initial conditions, atmospheric forcing, and model parameters, rather than only  
57 the initial conditions as in statistical-based methods. The resulting reanalysis completely follows the model governing  
58 equations without having to consider artificial source/sink terms.

59 Despite the application of the coupled ocean and sea ice adjoint model in sensitivity studies (Heimbach et al., 2010;  
60 Kauker et al., 2009; Koldunov et al., 2013) and reanalyses (Fenty and Heimbach, 2013; Koldunov et al., 2017; Lyu et  
61 al., 2021b; Nguyen et al., 2021), we have to omit the adjoint of sea ice dynamics (Fenty et al., 2017; Nguyen et al.,  
62 2021) or simplify it to the adjoint of a free-drift sea ice model (Koldunov et al., 2017; Lyu et al., 2021b) to ensure  
63 numerical stability of the adjoint model. Toyoda et al. (2019) noted that further including the adjoint of sea ice  
64 rheology results in a much weaker evolution of sensitivity to sea ice velocity by  $O(10^2)$  in the central Arctic Ocean

65 than the adjoint of free-drift sea ice dynamics. It is expected that including the adjoint of sea ice rheology could better  
66 project the model-data misfits to the control variables and potentially improve the quality of the reanalysis.

67 In this study, we incorporate and stabilise the adjoint of a viscous-plastic sea ice dynamic (Hibler, 1979; Zhang and  
68 Hibler 1997), building on prior developments of the coupled Arctic ocean and sea ice model and assimilation system  
69 (Koldunov et al., 2017; Lyu et al., 2021b). Using the unprecedented sea ice retreat process in 2012 as an example, we  
70 evaluate the impacts of using the approximated adjoint of viscous-plastic sea ice dynamics on estimating the Arctic  
71 ocean, sea ice, and sea-ice retreat processes.

72 The paper is organised as follows. In Section 2, we introduce the model configurations and assimilation  
73 experiments. We assess the assimilation results in terms of the residual errors in Section 3. We examine adjustments  
74 of the control variables in Section 4 and compare the sea ice retreat process in the assimilation runs in Section 5.  
75 Section 6 summarises the results of this study and discusses the potential for a further development of global and  
76 Arctic state and parameter estimation systems.

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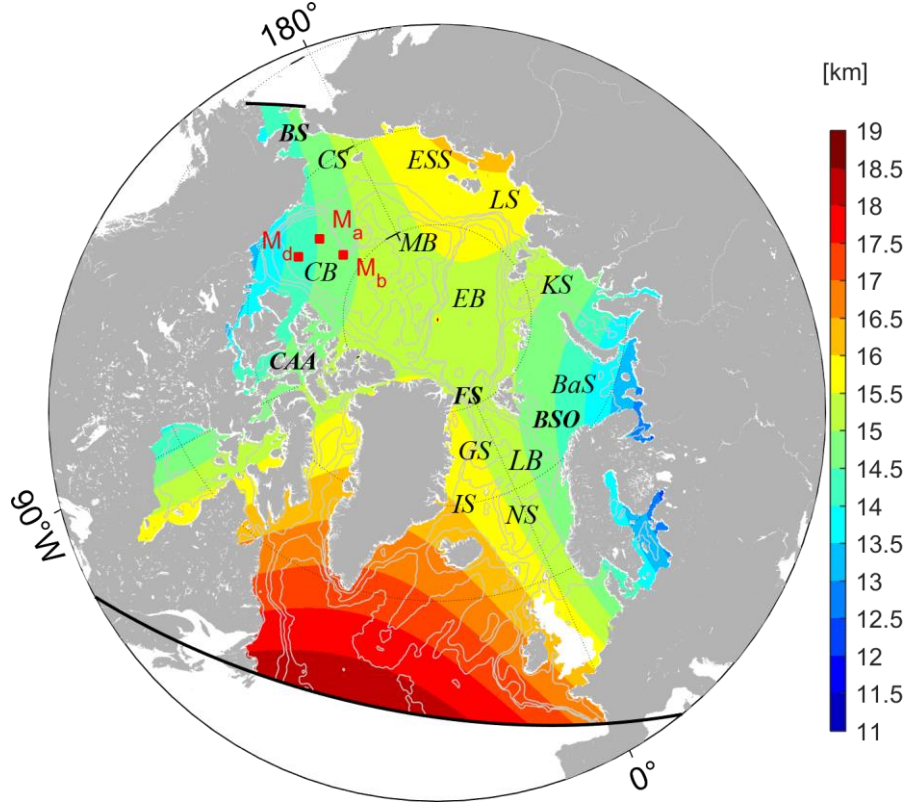
## 78 **2 Model Configuration and Experiment Setups**

### 79 **2.1 The Coupled Ocean and Sea Ice Modelling and Assimilation System**

80 The data assimilation system is based on the adjoint method in the ECCO framework, using the Massachusetts  
81 Institute of Technology ocean general circulation model (MITgcm, Marshall et al., 1997) coupled with the zero-layer  
82 dynamic-thermodynamic sea ice model of Hibler (1979). The sea ice dynamics are based on a viscous-plastic sea ice  
83 rheology and are solved using a line successive over-relaxation algorithm (Zhang and Rothrock, 2000). The  
84 thermodynamic sea ice model includes a prescribed sub-grid ice thickness distribution with 7 thickness categories. On  
85 top of the ice, a diagnostic snow model is applied which modifies the heat flux and surface albedo, as in Zhang and  
86 Rothrock (2000). The thermodynamic-dynamic sea ice model simulates changes in sea ice drift (SID), sea ice  
87 concentration (SIC), and mean sea ice thickness (in volume per unit area, mean SIT hereinafter). Losch et al. (2010)  
88 reformulated the sea ice model on an Arakawa C grid to match the MITgcm oceanic grid and modified the model  
89 codes to permit efficient and accurate automatic differentiation. The adjoint of the coupled ocean and sea ice model  
90 is generated by the Transformation of Algorithms in FORTRAN (TAF, Giering and Kaminski, 1998).

91 The pan-Arctic model covers the Arctic Ocean north of the Bering Strait and the Atlantic Ocean at 44° N  
92 (enclosed by black lines in Figure 1). In the horizontal direction, we use a curvilinear grid with a resolution of 12~15  
93 km in the Arctic Ocean and ~18 km in the North Atlantic Ocean. In the vertical direction, the system has 50 z-levels  
94 ranging from 10 m at the surface to 456 m in the deep ocean. The open boundaries are provided by a 16 km Atlantic-  
95 Arctic Ocean simulation (Serra et al., 2010). At the ocean surface, we use the atmosphere state from the National  
96 Centers for Environmental Prediction reanalysis 1 (NCEP-RA1, Kalnay et al., 1996) and bulk formulae (Large and  
97 Yeager, 2004) to compute the momentum, heat, and freshwater fluxes. A virtual salt flux parameterisation simulates  
98 the dilution and salinification of rainfall, evaporation, and river runoff. River runoff is applied near the river mouth  
99 with seasonally varying discharge (Fekete et al., 2002). In addition, unresolved vertical mixing is parameterised using  
100 the K-Profile scheme of Large et al. (1994). The background coefficients of vertical diffusion and viscosity are set to

101  $10^{-5} \text{m}^{-2} \text{s}^{-1}$  and  $5.6 \times 10^{-4} \text{m}^{-2} \text{s}^{-1}$ , respectively. Biharmonic viscosity with a coefficient of  $2.2 \times 10^{11} \text{m}^4 \text{s}^{-1}$  represents  
 102 unresolved sub-grid eddy mixing. The bottom topography is derived from ETOPO2 (Smith and Sandwell, 1997).



103 Figure 1. Map of the pan-Arctic regions showing the model domain (enclosed by the black lines) and horizontal  
 104 resolutions (shading). The red rectangles show the three moorings ( $M_a$ ,  $M_b$ ,  $M_d$ ) from the Beaufort Gyre Exploration  
 105 Project (BGEP). Major basins and straits are labelled as follows: Canada Basin ( $CB$ ), Makarov Basin ( $MB$ ), Eurasian  
 106 Basin ( $EB$ ), Chukchi Sea ( $CS$ ), East Siberian Sea ( $ESS$ ), Laptev Sea ( $LS$ ), Kara Sea ( $KS$ ), Barents Sea ( $BaS$ ), Greenland  
 107 Sea ( $GS$ ), Lofoten Basin ( $LB$ ), Iceland Sea ( $IS$ ), Norwegian Sea ( $NS$ ), Bering Strait ( $BS$ ), Fram Strait ( $FS$ ), Barents  
 108 Sea Opening ( $BSO$ ), and Canadian Arctic Archipelago ( $CAA$ ).  
 109

110  
 111 The adjoint method brings the model simulation close to available observations by iteratively adjusting control  
 112 variables to minimise a quadric target function  $J$  (cost function hereinafter):

$$113 J(C_{ini}, C_{atm}(t)) = \sum_{t=1}^{T_1} [y(t) - E(t)x(t)]^T R^{-2} [y(t) - E(t)x(t)] + C_{ini}^T P^{-2} C_{ini} + \sum_{t=0}^{T_1} C_{atm}(t)^T Q_a^{-2} C_{atm}(t) \quad (1).$$

114 On the right hand of Equation (1), the first term measures the model-data misfits weighted by the inverse error  
 115 covariance matrices ( $R^{-2}$ ). The following section will introduce the available measurements and their uncertainties ( $R$ ).  
 116  $y(t)$  and  $x(t)$  are observations and the model state at time  $t$ , respectively.  $E(t)$  maps the model state  $x(t)$  to the  
 117 corresponding observations  $y(t)$ . The last two terms are background terms of the initial condition ( $C_{ini}$ ) and the time-  
 118 varying atmospheric forcing ( $C_{atm}(t)$ ) weighted by their inverse error covariance matrices ( $P^{-2}$  and  $Q_a^{-2}$ , respectively),  
 119 which penalise their adjustments and provide complete information on the controls. Following Lyu et al. (2021b),  
 120 prior uncertainties of the time-varying atmosphere state ( $Q_a$ ) depend on geographic locations. They are computed as  
 121 the variance of the nonseasonal variability of the corresponding variables using NCEP-RA1.

122 For simplicity and the robust performance of this coupled data assimilation system, we choose the initial  
 123 conditions ( $C_{ini}$ ), including temperature, salinity, mean SIT, SIC, and daily atmosphere state on the model grid ( $C_{atm}(t)$ ),

124 which includes 10-m wind vectors, 2-m air temperature, 2-m specific humidity, precipitation, downwelling longwave,  
 125 and net shortwave radiation, as the control variables. In the future development of ocean and sea ice state estimation  
 126 systems, we further include the river runoff, the open boundary conditions, and model uncertain parameters as control  
 127 variables as in previous studies (e.g., Fenty and Heimbach, 2013; Liu et al., 2012). In this study, we use a one-year  
 128 assimilation window covering the year 2012, resulting in a total number of  $\sim 2.7 \times 10^8$  control variables.

129 During the optimisation process, the adjoint of the coupled ocean-ice model is used to compute the gradients of  
 130 the cost function  $J$  to the control variables, and a quasi-Newton algorithm (Gilbert and Lemaréchal, 2006) is used to  
 131 iteratively reduce the cost function  $J$ . The optimisation process continues until the cost function cannot be further  
 132 reduced.

## 133 2.2 Observations and Prior Uncertainties

134 Both satellite and in situ measurements (Table 1) are used to constrain the model simulations. In addition, sea ice  
 135 draft measurements by up-looking sonar from the Beaufort Gyre Exploration Project (BGEP, see Figure 1 for the  
 136 locations) are used to independently validate the assimilation results.

137 Prior uncertainties are detailed in our previous Arctic synthesis study (Lyu et al., 2021b). Uncertainties in  
 138 temperature and salinity depend on the depth and are set to 0.6 °C and 0.3 PSU at the surface and 0.02 °C and 0.02  
 139 PSU in the deep ocean; SIC uncertainties consist of representation errors (15% within 50 km from the coastlines and  
 140 10% over the open water) and instrument errors. Because of higher errors in low SIC and lower errors over open water,  
 141 we modify the representation uncertainties by multiplicative factors of 0.85, 1.20, 1.10, and 1.00 for the observed SIC  
 142 ranges of 0.00, <15%, 15%–25%, and 0.25%, respectively.

143 SIT errors are provided by the datasets and interpolated to our model grid. Sea level anomaly (SLA) uncertainties  
 144 are set to 3.0 cm. SID uncertainties are dominated by representation errors and are set to 0.04 m/s. Sea surface  
 145 temperature (SST) uncertainties are provided by the datasets. In addition, we reduce the weight of the temperature and  
 146 salinity climatology (WOA18) cost components by factors of 20.0 and 10.0, respectively, to avoid overfitting to the  
 147 climatology.

148 **Table 1.** Assimilated measurements.

Date sets	Resolution	Number	Source
Sea level anomaly	7.0 km	$7.6 \times 10^5$	Copernicus Marine Environment Monitoring Service, <a href="http://marine.copernicus.eu">http://marine.copernicus.eu</a>
Sea surface temperature	25.0 km	$2.0 \times 10^7$	Remote Sensing System, <a href="http://www.remss.com/measurements/sea-surface-temperature/">http://www.remss.com/measurements/sea-surface-temperature/</a>
T&S profiles	–	$5.0 \times 10^5$	Good et al. (2013), <a href="https://www.metoffice.gov.uk/hadobs/en4/">https://www.metoffice.gov.uk/hadobs/en4/</a>
Sea ice concentration	25.0 km	$3.6 \times 10^7$	Kaleschke et al. (2001) and Spreen et al. (2008), SSM/I (2011–2012), <a href="http://icdc.cen.uni-hamburg.de/1/daten/cryosphere.html">http://icdc.cen.uni-hamburg.de/1/daten/cryosphere.html</a>
Sea ice thickness	25.0 km	$8.9 \times 10^6$	Ricker et al. (2017), <a href="https://spaces.awi.de/pages/viewpage.action?pageId=291898639">https://spaces.awi.de/pages/viewpage.action?pageId=291898639</a>
Sea ice drift	62.5 km	$5.8 \times 10^5$	Lavergne et al. (2019), <a href="https://osi-saf.eumetsat.int/products/osi-405-c">https://osi-saf.eumetsat.int/products/osi-405-c</a>
WOA18	1.0°	$2.9 \times 10^7$	Zweng et al. (2018), <a href="https://www.nodc.noaa.gov/OC5/woa18/woa18data.html">https://www.nodc.noaa.gov/OC5/woa18/woa18data.html</a>

## 149 2.3 Viscous-Plastic Sea Ice Dynamics and Its Adjoint

150 In the coupled ocean and sea ice model, the following equation governs sea ice drift:

151 
$$m \frac{d\vec{u}}{dt} = -mf\vec{k} \times \vec{u} + \tau_{air} + \tau_{ocn} - \nabla\phi(0) + \nabla \cdot \sigma \quad (2)$$

152 where  $m$  is the sea ice mass and  $\vec{u}$  is the sea ice motion vector;  $\tau_{air}$  and  $\tau_{ocn}$  are the wind and ocean drags,  
 153 respectively;  $-\nabla\phi(0)$  is the tilt of the sea surface; and  $\nabla \cdot \sigma$  is the divergence of the ice stress tensor  $\sigma_{ij}$  ( $i=1,2$ ),  
 154 representing the internal forces of sea ice.

155 In the viscous-plastic rheology of Hibler (1979), the stress tensor  $\sigma_{ij}$  is related to the sea ice strain rate ( $\epsilon_{ij}$ ) and  
 156 strength ( $P$ ):

157 
$$\sigma_{ij} = 2\eta(\epsilon_{ij}, P)\epsilon_{ij} + [\zeta(\epsilon_{ij}, P) - \eta(\epsilon_{ij}, P)]\epsilon_{kk}\delta_{ij} - \frac{P}{2}\delta_{ij} \quad (3)$$

158 where  $\delta_{ij}$  is the Kronecker delta ( $\delta_{ij} = 1$  if  $i=j$ , otherwise 0).  $\eta$  and  $\zeta$  are the bulk and shear viscosities, expressed  
 159 as:

160 
$$\zeta = \frac{P}{2\Delta_{reg}} \quad (4)$$

161 
$$\eta = \frac{P}{2e^2\Delta_{reg}} \quad (5)$$

162 where

163 
$$\Delta = [(\epsilon_{11}^2 + \epsilon_{22}^2)(1 + e^{-2}) + 2(1 - e^{-2})\epsilon_{11}\epsilon_{22} + 4e^{-2}\epsilon_{12}^2]^{\frac{1}{2}} \quad (6)$$

164  $e$  is the ratio of normal stress to shear stress and is set to 2.0;  $\Delta_{reg} = \max(\Delta, \Delta_{min})$  with  $\Delta_{min}$  equals  $1.0 \times 10^{-10}$ . The  
 165 sea ice strain rate is computed as:

166 
$$\epsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (7).$$

167 The sea ice strength  $P$  depends on mean SIT ( $H$ ) and SIC ( $C$ ):

168 
$$P = P^*H \cdot \exp(-C^* \cdot (1 - C)) \quad (8)$$

169  $P^*$  and  $C^*$  are the ice compressive strength constant and ice strength decay constant and are set to  $2.75 \times 10^4 \text{ N m}^{-2}$   
 170 and -20.0, respectively.

171 The dependence of the internal force term ( $\nabla \cdot \sigma$ ) on ice velocity is strongly nonlinear, leading to an unstable  
 172 adjoint of the coupled ocean-sea ice system. Therefore, previous studies (Koldunov et al., 2017; Lyu et al., 2021b)  
 173 used an adjoint of a free drift sea ice model (without an adjoint of  $\nabla \cdot \sigma$ ). Toyoda et al. (2019) pointed out that the full  
 174 adjoint of Equation (2) can be stabilised by eliminating the dependence of bulk and shear viscosities on the strain rate  
 175 ( $\epsilon_{ij}$ ).

176 Following the study of Toyoda et al. (2019), we eliminate the dependence of bulk and shear viscosities on  $\epsilon_{ij}$  in  
 177 the adjoint of Equation (2). In addition, we note that there are still strong sensitivities that hamper the convergence of  
 178 optimization. We set the adjoint sensitivities of ice velocity to zero if the local sensitivity is 50 times larger than the  
 179 global mean of their absolute values. In addition, we also modify the adjoint model in the following ways to ensure  
 180 the stability of the adjoint model over a one-year assimilation window:

181 1) Disable the K-profile mixing parameterisation scheme;

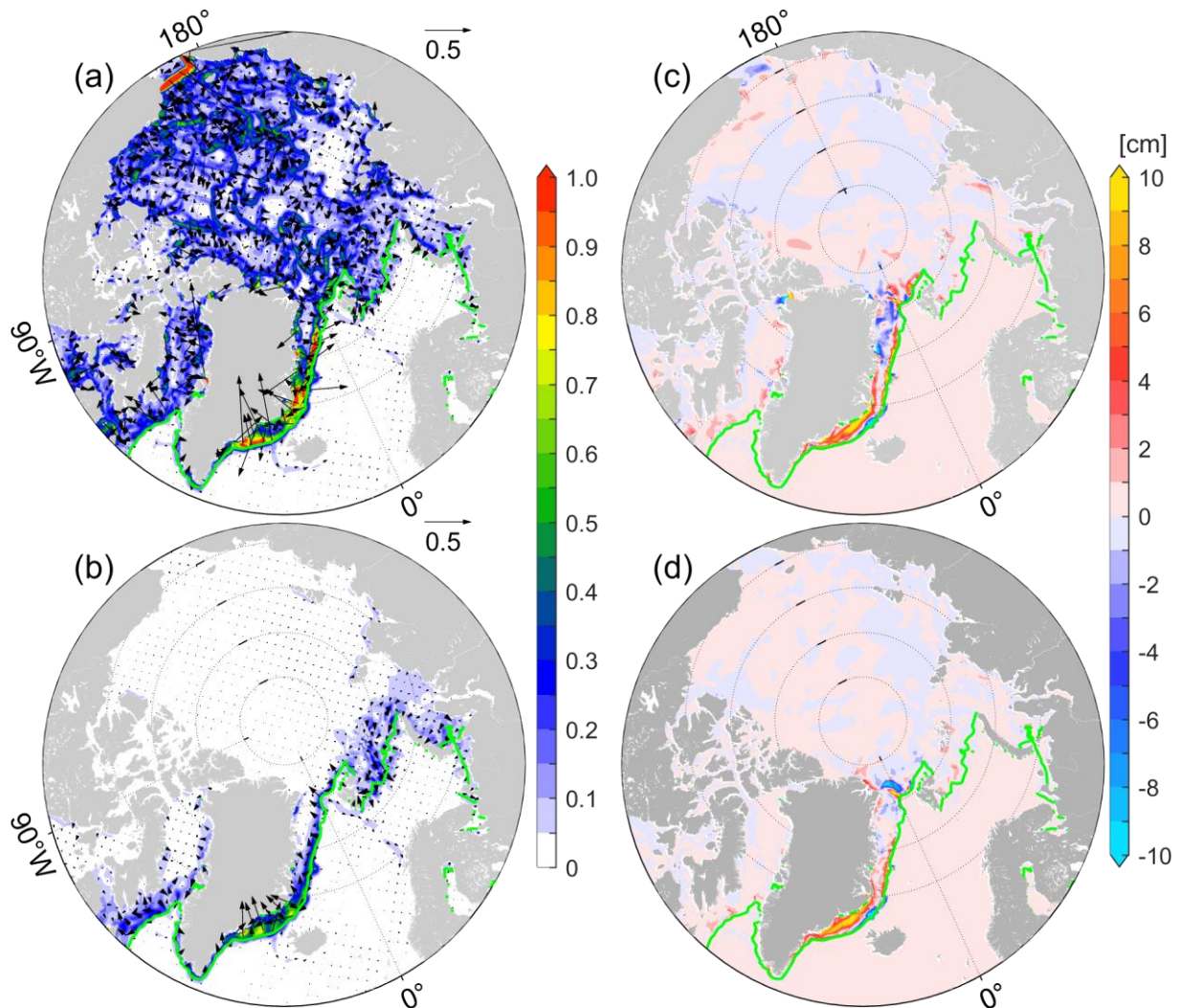
182 2) Increase the Laplacian diffusivity of heat and salinity to  $500 \text{ m}^2 \text{ s}^{-1}$  and lateral eddy viscosity to  $10,000 \text{ m}^2 \text{ s}^{-1}$ ;

183

184 3) Apply a spatial filter to sensitivity variables calculated in the adjoint of the thermodynamic sea ice model  
185 (see APPENDIX in Lyu et al. (2021b) for details).

186 Since the sea ice dynamic model is solved using an iterative line successive over-relaxation solver, we note that  
187 the approximated adjoint of the viscous-plastic sea ice dynamic (adjoint-VP) requires  $\sim 1.2$  times the computational  
188 cost of using the adjoint of a free-drift sea ice model (adjoint-FD).

189



190

191 Figure 2. Sensitivities of total sea ice volume to wind vectors (in  $0.1 \times \text{km}^3 (\text{m s}^{-1})^{-1}$ , shadings represents amplitudes)  
192 using the adjoint of (a) a free-drift sea ice dynamic and (b) viscous-plastic sea ice dynamics with modifications in  
193 Section 2.3. Panels (c)-(d) show the mean SIT changes by perturbing the wind with the corresponding adjoint  
194 sensitivities multiplied by a factor of  $10^{-8}$ . The green lines are the sea ice extents (SIEs, 15% SIC) in January 2012.  
195

196 Based on adjoint-FD and adjoint-VP, we compute the sensitivities of domain-integrated sea ice volume with  
197 respect to the atmospheric forcings and the initial conditions over the period of January 1 to January 31, 2012. As  
198 reported by Toyoda et al. (2019), adjoint-FD shows much stronger sensitivities to wind than does adjoint-VP (Figure  
199 2a, b) in the central Arctic Ocean. Along the sea ice marginals (SIMs) of the Atlantic sectors, adjoint-VP reveals that  
200 the towards-ice wind anomalies increase total sea ice (Figure 2b) since they prevent ice from drifting to the warm

201 Atlantic water. However, adjoint-FD shows strong sensitivities along the SIMs of the Atlantic sectors, but both  
 202 towards-ice and off-ice wind anomalies appear (Figure 2a), potentially resulting in ice convergence.

203 Furthermore, we add daily wind perturbations, computed by scaling the adjoint sensitivities (Figure 2a, b) so that  
 204 the maximum perturbations are  $1.0 \text{ m s}^{-1}$ , to the 6-hourly wind from NCEP-RA1 and examine their impacts on mean  
 205 SIT changes. As expected, mean SIT changes are mainly along the SIMs in the Atlantic sectors (Figure 2c, d), and  
 206 wind perturbations from adjoint-FD reduces mean SIT northeast of Greenland (Figure 2c). In the central Arctic Ocean  
 207 with compact ice, the internal forces  $\nabla \cdot \sigma$  oppose the impacts of wind perturbations. Therefore, despite the strong  
 208 adjoint sensitivities to the wind in adjoint-FD, we note that the resulting wind perturbations only slightly change the  
 209 mean SIT (Figure 2c), which is comparable to that in adjoint-VP (Figure 2d).

210 In addition to overestimating the sensitivities to wind, adjoint-FD may degrade the usefulness of the adjoint  
 211 sensitivities in optimisation. Therefore, we perform two assimilation experiments to comprehensively evaluate the  
 212 impacts of including the approximate adjoint of sea ice rheology on ocean and sea ice estimations.

### 213 3 Model-Data Misfit Reductions and Residuals

#### 214 3.1 Evaluation of the Optimisation

215 In this study, we consider iteration 0 the control run. In adjoint-FD and adjoint-VP, the optimisations stall at  
 216 iterations 13 and 32, and the further cost function reductions at the last two successive iterations are 0.7% and 0.2%  
 217 of the total cost, respectively. After the optimisations, the total cost and norms of the gradients are reduced by 32.3%  
 218 and 59.2% , respectively, in adjoint-FD and by 40.2% and 89.3%, respectively, in adjoint-VP.

219 **Table 2.** Normalised costs and reductions in the two optimisation runs.

<i>Cost constituent</i>	<b>Control run</b>	<b>Adjoint-FD</b>		<b>Adjoint_VP</b>	
	Normalised cost (%)	Normalised cost (%)	Percentage reduction (%)	Normalised cost (%)	Percentage reduction (%)
$J_{Total}$	100	67.7	32.3	59.8	40.2
$J_{SLA}$	2.2	2.1	4.6	2.1	4.6
$J_{SST}$	25.3	15.4	39.1	12.9	49.0
$J_{profile\_T}$	6.9	6.5	5.8	4.3	37.7
$J_{profile\_S}$	5.8	5.9	-1.7	4.5	22.4
$J_{SIC}$	39.7	18.4	53.7	18.1	54.4
$J_{SIT}$	3.6	3.1	13.9	2.7	25.0
$J_{SID}$	4.5	4.4	2.2	4.3	4.4
$J_{WOA\_T}$	6.6	6.6	0.0	6.2	6.1
$J_{WOA\_S}$	5.4	5.3	1.9	4.7	13.0

220  
 221 Of the individual cost constituents (Table 2), satellite-observed SST ( $J_{SST}$ ) and SIC ( $J_{SIC}$ ) contribute ~25.3% and  
 222 39.7% of the total cost, respectively, which are significantly reduced after optimisation. The costs of the temperature  
 223 ( $J_{profile\_T}$ ) and salinity ( $J_{profile\_S}$ ) profiles are also considerably reduced, especially in the adjoint-VP. The rest of the cost  
 224 constituents are also slightly reduced. Overall, including the adjoint of sea ice rheology further reduces the total cost  
 225 by 7.9% and the individual cost constituents, especially  $J_{sst}$ ,  $J_{profile\_T}$  and  $J_{profile\_S}$ . Based on iterations 0, and 13 in  
 226 adjoint-FD, and 32 in adjoint-VP of the optimisation, we will focus on the sea ice state and ocean temperature to  
 227 evaluate the impacts of using this approximate adjoint of sea ice rheology.

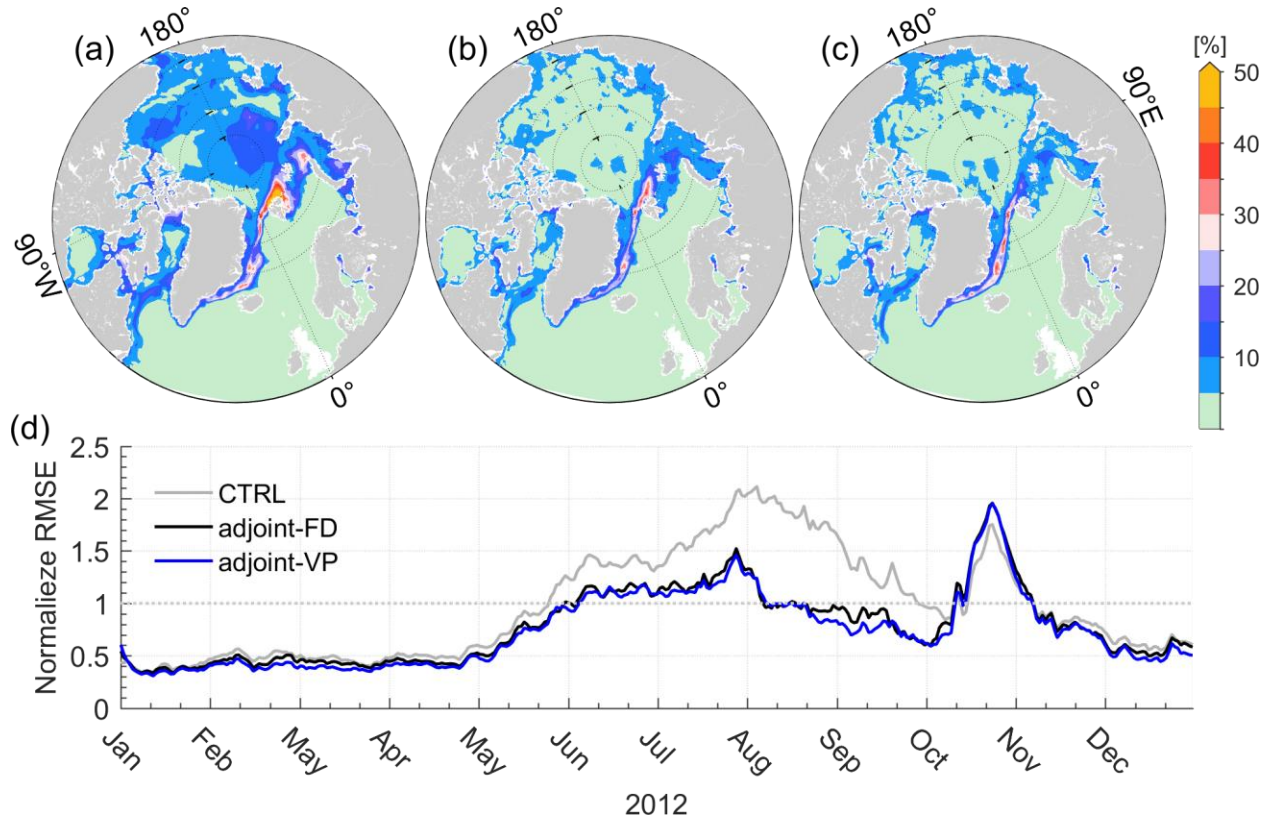
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229 **3.2 Sea Ice State**

230 **3.2.1 Residual Errors of SIC and SIT**

231 Satellite visual, infrared, and microwave technologies have been applied to monitor SIC with high frequencies  
232 and quality, which is of high priority in global and Arctic-focused synthesis (Chevallier et al., 2017; Uotila et al.,  
233 2019). Previous studies (Fenty and Heimbach, 2013; Lyu et al., 2021a; Lyu et al., 2021b) indicated that SIC could be  
234 significantly improved by slightly adjusting the atmospheric forcings. Here, we explore the residual errors in the  
235 optimisation runs.



236

237 Figure 3. Root mean square errors (RMSEs) of SIC between the satellite measurements and (a) the control run, (b)  
238 adjoint-FD, and (c) adjoint-VP averaged over 2012. Panel (d) shows the temporal variations in RMSEs normalised by  
239 prior uncertainties in the three simulations averaged over the sea ice-covered regions.

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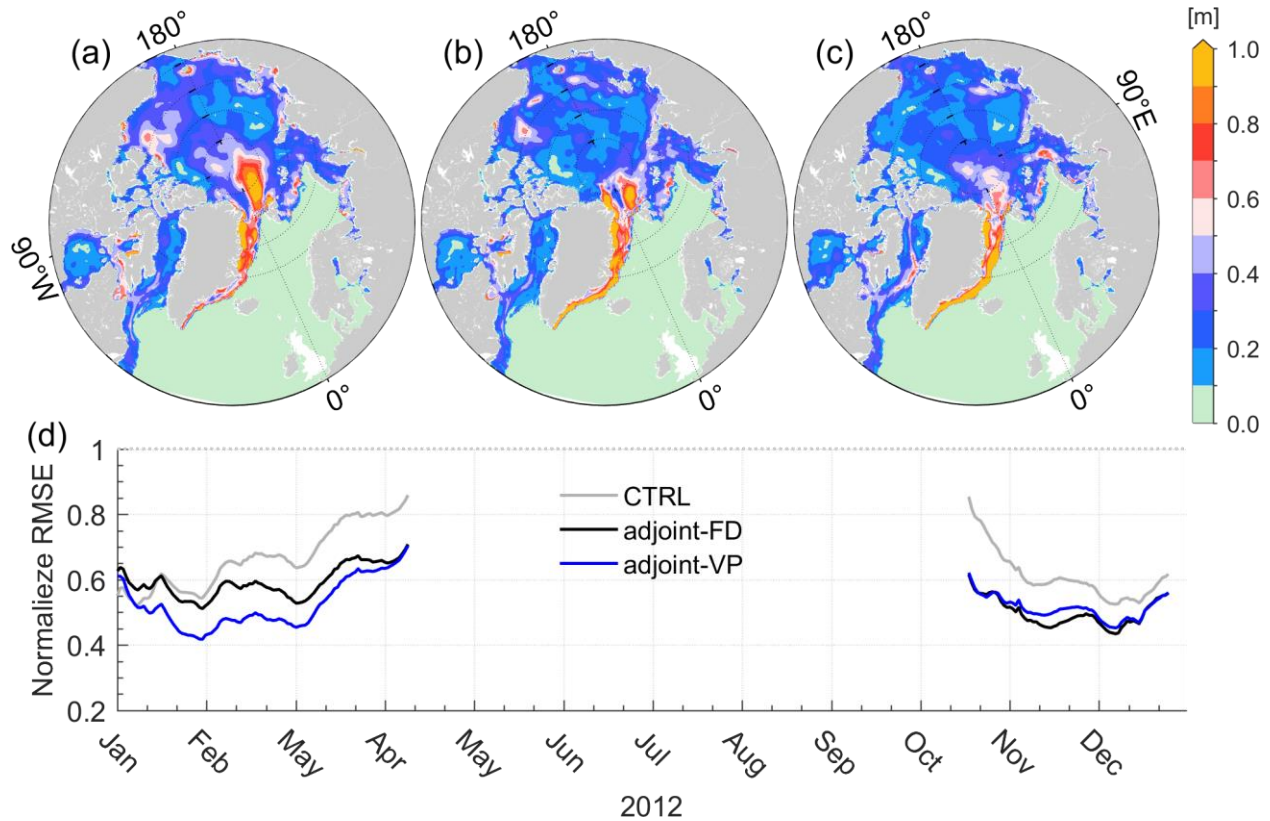
241 The root mean square errors (RMSEs) of SIC averaged over 2012 (Figure 3a-c) and normalised by the prior  
242 errors and averaged over the model domain (Figure 3d) show the geographical distribution and temporal evolution of  
243 SIC errors, respectively. The normalised RMSEs in Figure 3d should be close to 1.0 if the optimisation found a model  
244 simulation consistent with the observations and the prior uncertainties.

245

246 The control run (Figure 3a) shows pronounced RMSEs in the Beaufort Gyre (~15%), the central Eurasian Basin  
247 (15%~20%), the marginal seas (15%~20%), and SIMs of the Atlantic sector (30%-50%). The normalised RMSEs  
248 reveal that SIC errors remain small (~0.5) in the winter time (Figure 3d), indicating that the control run and the satellite  
SIC measurements match well, but they grow quickly from May-September when the sea ice melts (Figure 3d).

249 Normalised RMSEs up to 1.5 are observed in October but quickly drop in November (Figure 3d). Therefore, SIC  
 250 errors are significant during the melting and refreezing periods (from May to November).

251 Both assimilation experiments reduce the SIC errors to less than 5% in the central Arctic Ocean and 10% in the  
 252 marginal seas. SIC errors of up to 20% persist in the Atlantic sector, where sea ice shows strong nonlinearity and the  
 253 tangent linear model can capture only part of the sea ice changes (APPENDIX B in Lyu et al., 2021a). Normalised  
 254 SIC errors from May to September are also reduced to close to 1.0 by assimilation of the daily SIC observations  
 255 (Figure 3d). However, SIC errors in October remain significant (Figure 3d) since the observed sea ice recovers much  
 256 faster than in the control run and the two assimilation runs (not shown here). This delayed sea ice recovery in the  
 257 model may be related to model uncertain parameters, such as the threshold thickness between thin and thick ice, which  
 258 determines the initial sea ice thickness formed in open water.



259  
 260 Figure 4. Root mean square errors (RMSEs) of SIT between the satellite measurements and (a) the control run, (b)  
 261 adjoint-FD, and (c) adjoint-VP averaged over 2012. Panel (d) shows the temporal variations in RMSEs normalised by  
 262 prior uncertainties in the three simulations averaged over the sea ice-covered regions.  
 263

264 The control run shows SIT errors of up to 1.0 m in regions north and south of the Fram Strait and approximately  
 265 0.4~0.7 m in the Beaufort Gyre. In the Beaufort Gyre, the SIT errors are reduced to less than 0.3 m in adjoint-VP  
 266 (Figure 4c) and approximately 0.3-0.5 m in adjoint-FD (Figure 4b). Similar to the SIC errors, SIT errors of up to 1.0  
 267 m remain along the East Greenland Current, which seems to increase in the two assimilation experiments. The  
 268 temporal evolutions of normalised RMSEs show that the SIT errors grow quickly from February to April (Figure 4d).  
 269 Both assimilation experiments reduce the SIT errors, especially in adjoint-VP from January to April (Figure 4d).

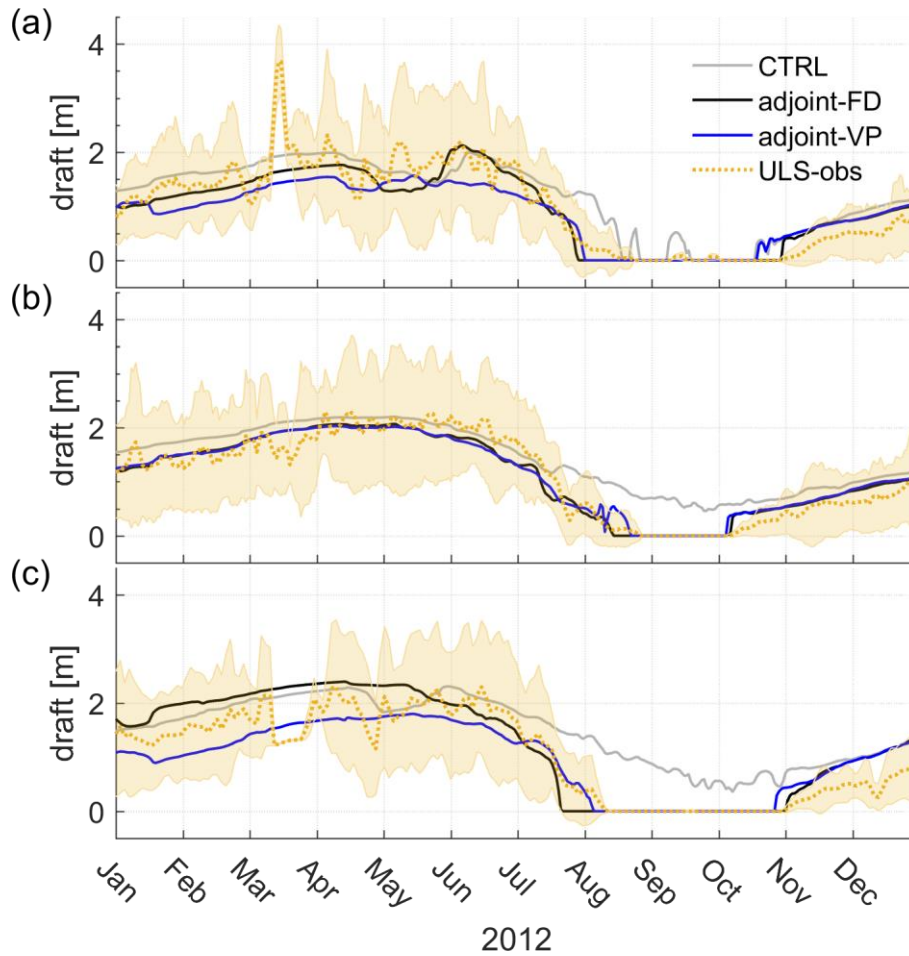
270 However, the normalised RMSEs of SIT averaged over the model domain remain smaller than 1.0 and seem to grow  
 271 during the melting season. More accurate SIT observations (e.g., half of the uncertainties) and SIT observations during  
 272 the melting season are required to facilitate a significant impact on the model simulation.

### 273 3.2.2 BGEF Mooring Measurements

274 Independent sea ice draft measured by up-looking-sonar (ULS) on the BGEF moorings ( $M_a$ ,  $M_b$ , and  $M_d$  in  
 275 Figure 1) is used to validate the simulated sea ice draft. The simulated snow depth ( $d_{snow}$ ) and SIT ( $d_{SIT}$ ) are used to  
 276 compute the sea ice draft following the methods of Tilling et al. (2018):

$$277 \text{draft} = \frac{\rho_i \times d_{SIT} + \rho_s \times d_{snow}}{\rho_w} \quad (9)$$

278 where  $\rho_i$ ,  $\rho_s$ , and  $\rho_w$  are the densities of the sea ice, snow, and water, respectively, and are set to 910.0, 330.0, and  
 279 1027.5 kg m<sup>-3</sup>, respectively, as in our model.



280  
 281 Figure 5. Daily time series of the sea ice draft (dotted yellow lines) and the daily standard deviation (shadings) at the  
 282 mooring locations (a)  $M_a$ , (b)  $M_b$ , and (c)  $M_d$  compared with the control run and the two assimilation runs (see the  
 283 legend) throughout the year 2012. ULS-observed sea ice drafts are smoothed with a 5-day running average.  
 284

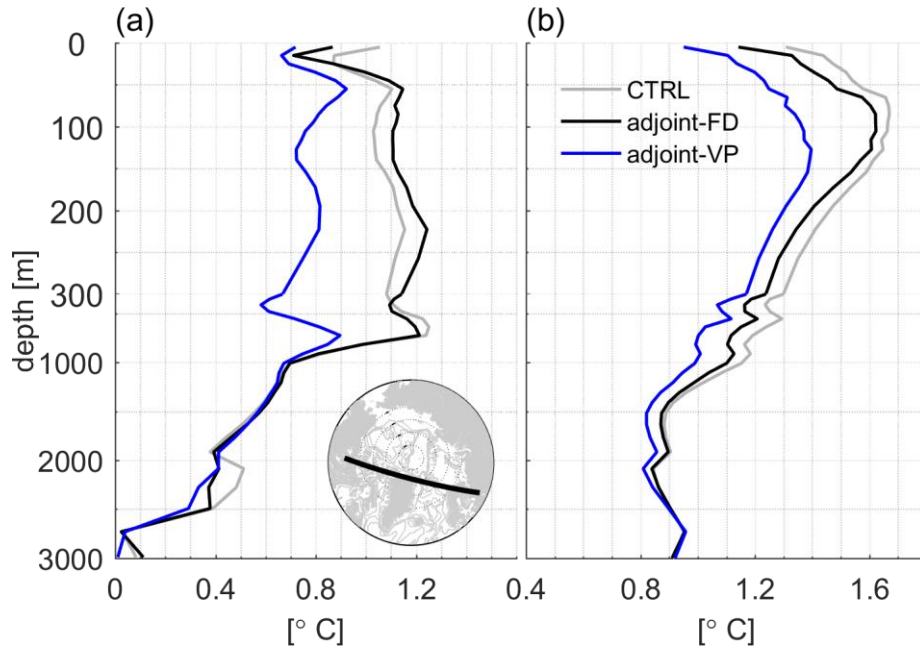
285 The ULS measurements depict stronger daily to sub-monthly sea ice draft variability than do the model  
 286 simulations, which may be related to ice floe motions. The control run simulates a delayed ice disappearance process

287 in  $M_a$  (Figure 5a) and fails to reproduce the sea ice disappearance processes in  $M_b$  (Figure 5b) and  $M_d$  (Figure 5c) from  
 288 August to October. After optimisation, adjoint-VP and adjoint-FD reproduce the sea ice melting and refreezing  
 289 processes well, although errors of up to 0.5 m remain from January to June. Overall, the two assimilation runs  
 290 reproduce the local sea ice retreat and recovery process well.

291

### 292 3.3 Ocean Temperature

293 Ocean temperature changes are closely related to sea ice changes. Adjoint-VP introduces more pronounced ocean  
 294 temperature changes than does adjoint-FD. Here, we explore ocean temperature changes after assimilation.



295  
 296

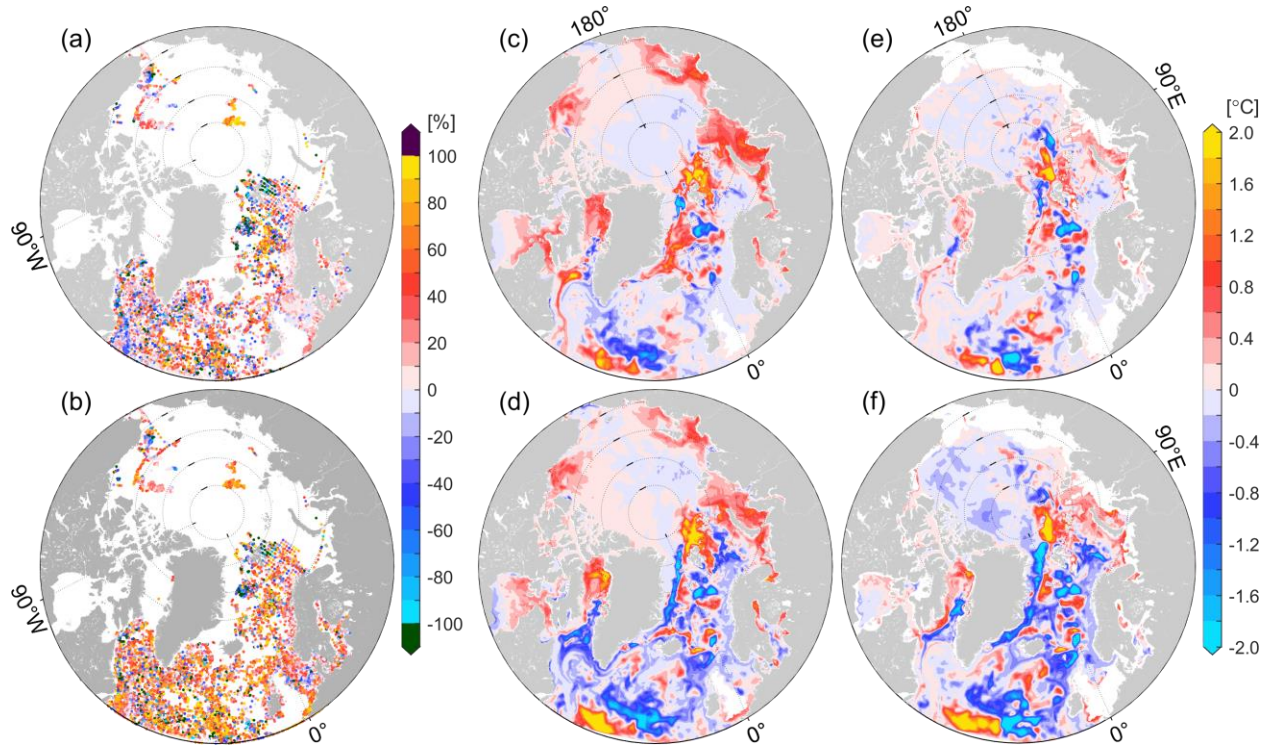
297 Figure 6. RMSEs of potential temperature (a) in the Arctic Ocean and (b) the North Atlantic Ocean in the three runs.  
 298 The Arctic Ocean and the North Atlantic Ocean are separated by the black lines in the bottom subplot.

299

300 In the Arctic Ocean, adjoint-FD reduces temperature errors only over the top 20 m, while adjoint-VP reduces  
 301 temperature errors up to 0.4 °C over the top 1000 m (Figure 6a). In the North Atlantic Ocean, adjoint-VP results in a  
 302 more pronounced RMSEs reduction up to 0.3 °C than adjoint-FD (Figure 6b).

303

304 Relative temperature error reductions over the top 50 m reveal an overall improvement in temperature with  
 305 occasional degradation (Figure 7a, b). Adjoint-VP results in a more significant error reduction than does adjoint-FD  
 306 in the North Atlantic Ocean (Figure 7a, b). In the southern Beaufort Gyre, the Laptev and Kara seas, and north of  
 307 Svalbard, both adjoint-VP and adjoint-FD increase the ocean temperature (over 50 m) since the two optimisation runs  
 308 reproduce the early retreat of the sea ice well, allowing more solar heating of the open water. In the North Atlantic  
 309 Ocean, adjoint-VP achieves more considerable temperature changes than does adjoint-FD both over the top 50 m  
 310 (Figure 7c, d) and from 50 m-700 m (Figure 7e, f). In the Arctic Ocean, adjoint-VP further introduces negative  
 311 temperature corrections between 50 and 700 m (Figure 7f), especially near the profile locations (see dots in Figure  
 7b).



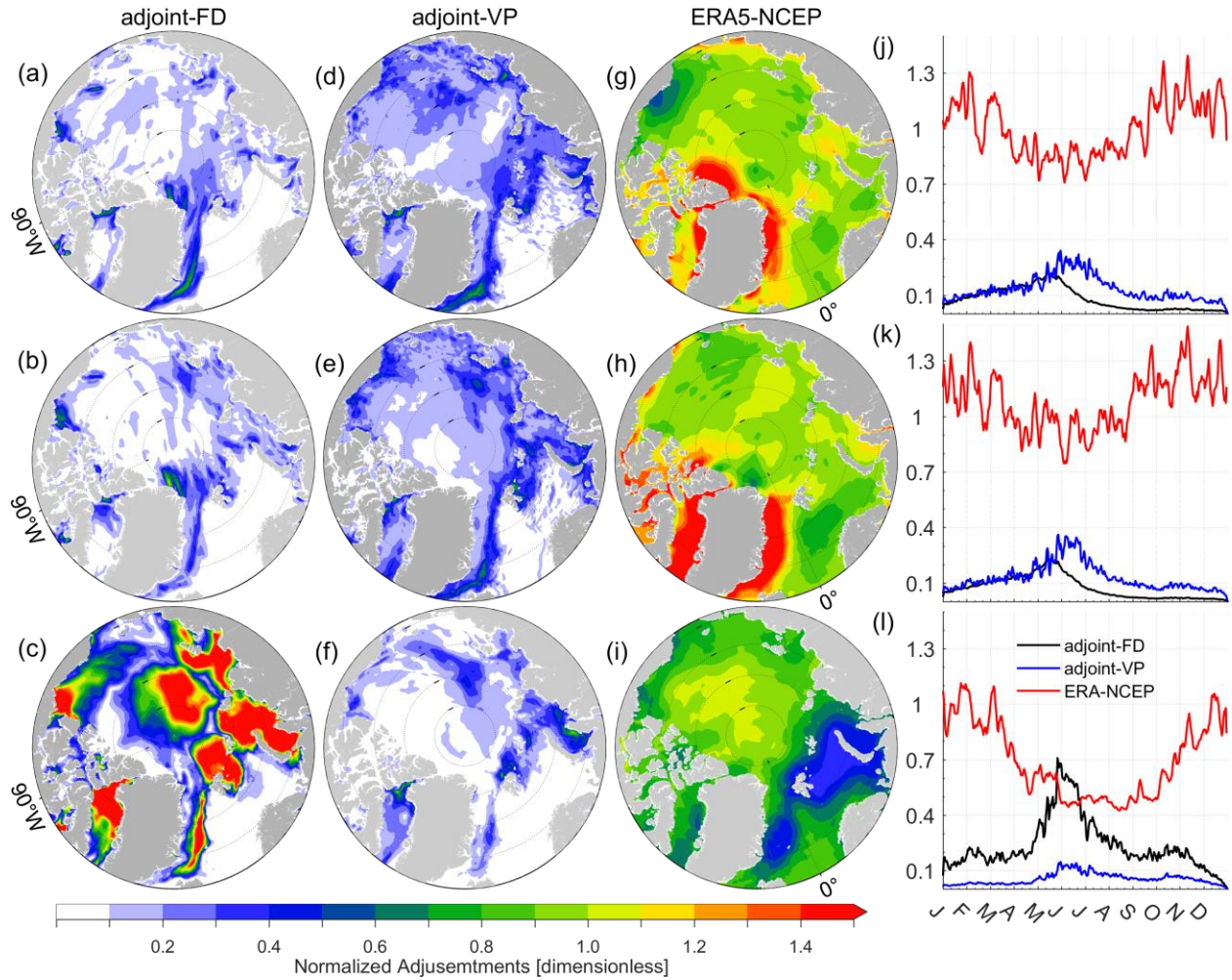
312  
 313 Figure 7. Relative temperature error reduction ( $-\frac{|T_{opti}-T_{obs}| - |T_{ctrl}-T_{obs}|}{|T_{ctrl}-T_{obs}|} \times 100\%$ ) over the top 50 m at the profile  
 314 locations in (a) adjoint-FD and (b) adjoint-VP. Values >100% indicate over-adjustment. Panels (c) and (d) show the  
 315 temperature differences of adjoint-FD and adjoint-VP to the control run averaged over the top 50 m, respectively.  
 316 Panels (e) and (f) are the same as Panels (c) and (d), but for the 50-700 m layers.  
 317

318 In summary, adjoint-FD and adjoint-VP reproduce the SIC variations well in the Arctic Ocean, which further  
 319 reduces ocean temperature errors in the top layer by improving the atmosphere-ocean heat flux. Adjoint-VP achieves  
 320 more significant corrections to the ocean temperature over the open water and in the intermediate layer of the Arctic  
 321 Ocean than does adjoint-FD.

#### 322 4 Adjustment of the Control Variables

323 The adjoint models project the model-data misfits onto the gradient of the objective function with respect to all  
 324 control variables simultaneously, which is used by the optimisation algorithm to adjust the control variables. In this  
 325 section, we compare adjustments of the control variables in the adjoint-FD and adjoint-VP and evaluate contributions  
 326 of individual adjustments of the control variables on the cost function reduction. We also compare the adjustments of  
 327 the control variables in adjoint-FD and adjoint-VP with differences between ERA5 (Hersbach et al., 2020) and NCEP-  
 328 RA1 reanalyses.

329 Among all the control variables, wind vectors and 2-m air temperature are considerably adjusted in adjoint-FD  
 330 and adjoint-VP but also show significant differences. In addition, adjoint-VP induces more pronounced adjustments  
 331 of the initial temperature and salinity than does adjoint-FD (not shown here). Here, we concentrate on the adjustments  
 332 of wind vectors and the 2-m air temperature.



333  
 334 Figure 8. Root mean square (RMS) of the adjustments of the (a) wind  $u$ -component, (b) wind  $v$ -component, and (c) 2-  
 335 m air temperature normalised by their prior uncertainties (dimensionless) in adjoint-FD and averaged over 2012.  
 336 Panels (d)-(f) are similar to (a)-(c) but for adjoint-VP. Panels (g)-(i) show the normalised RMS of differences in the  
 337 (g) wind  $u$ -component, (h) wind  $v$ -component, and (i) 2-m air temperature between ERA5 and NCEP-RA1 reanalyses  
 338 (normalised by prior uncertainties in assimilation experiments). Panels (j)-(l) are the area averages of the normalised  
 339 RMS of adjustments (differences) of the wind  $u$ -component, wind  $v$ -component, and 2-m air temperature  
 340 (dimensionless) in adjoint-FD and adjoint-VP (ERA5-NCEP).  
 341

342 Figure 8 shows the root mean square (RMS) of the adjustments of the wind vectors and 2-m air temperature  
 343 normalised by their prior uncertainties. The normalised RMS of the adjustments of the control variables should be  
 344 smaller than 1.0 if the adjustments are within their prior uncertainties. Adjoint-FD slightly adjusts the wind vectors  
 345 (with the normalised RMS of the adjustments being smaller than 0.4, Figure 8a, b), but the 2-m air temperature is  
 346 significantly adjusted (with the normalised RMS of adjustments being greater than 1.5, Figure 8c). In adjoint-VP,  
 347 the wind vectors and 2-m air temperature are slightly adjusted (Figure 8d-f) with their normalised RMS of  
 348 adjustments being smaller than 0.3. In addition to the different amplitudes of the adjustments, the maximum  
 349 adjustments of the wind vectors appear in June in adjoint-VP but in May in adjoint-FD (Figure 8j, k). Throughout  
 350 2012, the 2-m air temperature is adjusted more prominently in adjoint-FD than in adjoint-VP (Figure 8l).

351 We note that the adjustments of the three atmosphere state variables in Figure 8a-f resemble the SIC (Figure 3a)  
 352 and SIT (Figure 4a) error patterns, indicating that these adjustments are mostly determined by sea ice state errors that  
 353 are projected on the control variables by the adjoint models rather than the background terms (the second and third  
 354 terms on the right hand side of Equation (1)). Excluding the adjoint of sea ice rheology (adjoint-FD) results in over-  
 355 adjustments of 2-m air temperature. With an approximated adjoint of sea ice rheology (adjoint-VP), we reduce the  
 356 model-data misfits by slightly adjusting the control variables.

357 Using the new generation ERA5 reanalysis, we further compare the ERA5-NCEP differences against the  
 358 adjustments of the atmosphere state variables in terms of their spatial patterns and temporal variability. The purpose  
 359 of this comparison is twofold: 1) it further justifies the rationale of the adjustment amplitudes, and 2) it examines  
 360 whether the adjustments reflect the differences between the old generation NCEP-RA1 reanalysis and the new  
 361 generation ERA5 reanalysis. For the wind vectors, the normalised RMS differences between the ERA5 and NCEP-  
 362 RA1 reanalyses (Figure 8g, h) are much larger than the wind vector adjustments in adjoint-FD (Figure 8a, b) and  
 363 adjoint-VP (Figure 8d, e). For the 2-m air temperature, the normalised ERA5-NCEP differences ( $>1.0$ , Figure 8i) are  
 364 much larger than the normalised adjustments in adjoint-VP ( $<0.3$ , Figure 8f) but smaller than the normalised  
 365 adjustments in adjoint-FD ( $>1.5$ , Figure 8c) in the Kara Sea, the Laptev Sea, the southern Beaufort Sea, the Eurasian  
 366 Basin and the Makarov Basin. It is evident that the 2-m air temperature adjustments in adjoint-FD are too large.  
 367 Averaged over the model domain and throughout 2012, the ERA5-NCEP differences are much larger than the  
 368 adjustments (Figure 8j-l) in the two assimilation runs. In addition, the adjustments are larger from May to August  
 369 than from September to April, while the ERA5-NCEP differences are larger in the winter season than in the summer  
 370 season (Figure 8j-l). The comparisons confirm that the 2-m air-temperature is over-adjusted in adjoint-FD, especially  
 371 from May to July (Figure 8l). The adjustments of wind vectors and 2-m air temperature do not resemble the ERA5-  
 372 NCEP differences, indicating that the model-data differences cannot be fully fixed by replacing the old generation  
 373 NCEP-RA1 reanalysis with the new generation ERA5 reanalysis.

374

375 **Table 3.** Contributions of the adjustments of 2-m air temperature, wind vectors, initial temperature and salinity (Initial  
 376 T&S), and the remaining control variables (including initial mean SIT and SIC, 2-m specific humidity, precipitation,  
 377 downwelling longwave, and net shortwave radiation) on the total cost reduction, SIC, SST, and temperature profiles  
 378 in the two optimisation runs.

	Adjoint-FD (%)				Adjoint-VP (%)			
	2-m air temperature	Wind vectors	Initial T & S	Remaining variables	2-m air temperature	wind	Initial T & S	Remaining variables
$J_{total}$	29.0	17.5	6.0	3.0	5.3	52.6	25.1	5.0
$J_{SIC}$	25.5	19.8	2.4	1.2	4.5	64.9	10.1	2.4
$J_{SST}$	41.0	8.6	10.1	5.5	8.4	47.4	29.6	6.4
$J_{prof\_T}$	3.9	4.9	4.3	4.3	4.4	40.9	182.0	7.9

379

380 By replacing the adjusted initial temperature and salinity, wind vectors, 2-m air temperature, and the remaining  
 381 control variables with NCEP-RA1 datasets, we integrate the model and estimate the contributions of these variables  
 382 to the total cost reductions and individual components. Table 3 summarises contribution of individual control variables  
 383 to the total cost reductions and cost components of SIC, SST, and temperature profiles.

384 The small contributions of the adjustments of the remaining control variables (“Remaining variables” in Table 3)  
 385 to the cost function reductions in adjoint-FD and adjoint-VP highlight the importance of simultaneous adjustments of  
 386 the initial temperature and salinity, wind vectors and 2-m air temperature. In adjoint-FD, the adjustments of the 2-m  
 387 air temperature and wind vectors dominate the cost function reduction, especially the SIC components. In contrast,  
 388 adjoint-VP relies more on the adjustments of the wind vectors and the initial temperature and salinity. Besides, the  
 389 more pronounced ocean temperature improvements (see Figure 7) in adjoint-VP are mostly attributed to the  
 390 adjustments in the initial temperature and salinity (Table 3).

391 Overall, Adjoint-FD attributes more of the model-data misfits to the 2-m air temperature than does the adjoint-VP,  
 392 resulting in over-adjustments of the 2-m air temperature. By using an approximated adjoint of the sea ice rheology  
 393 (adjoint-VP), we reduce the model-data misfit by slightly adjusting the control variables. This leads to the conclusion  
 394 that the large 2-m air temperature adjustments in adjoint-FD is likely an overcompensation for wind errors that cannot  
 395 be appropriately corrected because of large errors in the respective cost function gradients.

### 396 **5 The Impacts on Sea Ice Retreat Processes**

397 A unique characteristic of the adjoint-based reanalysis is that its physical processes are described by the  
 398 governing equations of the model, allowing us to quantify the sea ice loss and the contributions of the sea ice dynamics  
 399 and sea ice-ocean-atmosphere fluxes through a closed budget analysis. In this section, we explore and compare the  
 400 mean SIT changes based on the model governing equation:

$$401 \quad \frac{dh}{dt} = -\nabla \cdot (\vec{u}h) + F_{oi} + F_{ai} + F_{res} \quad (10).$$

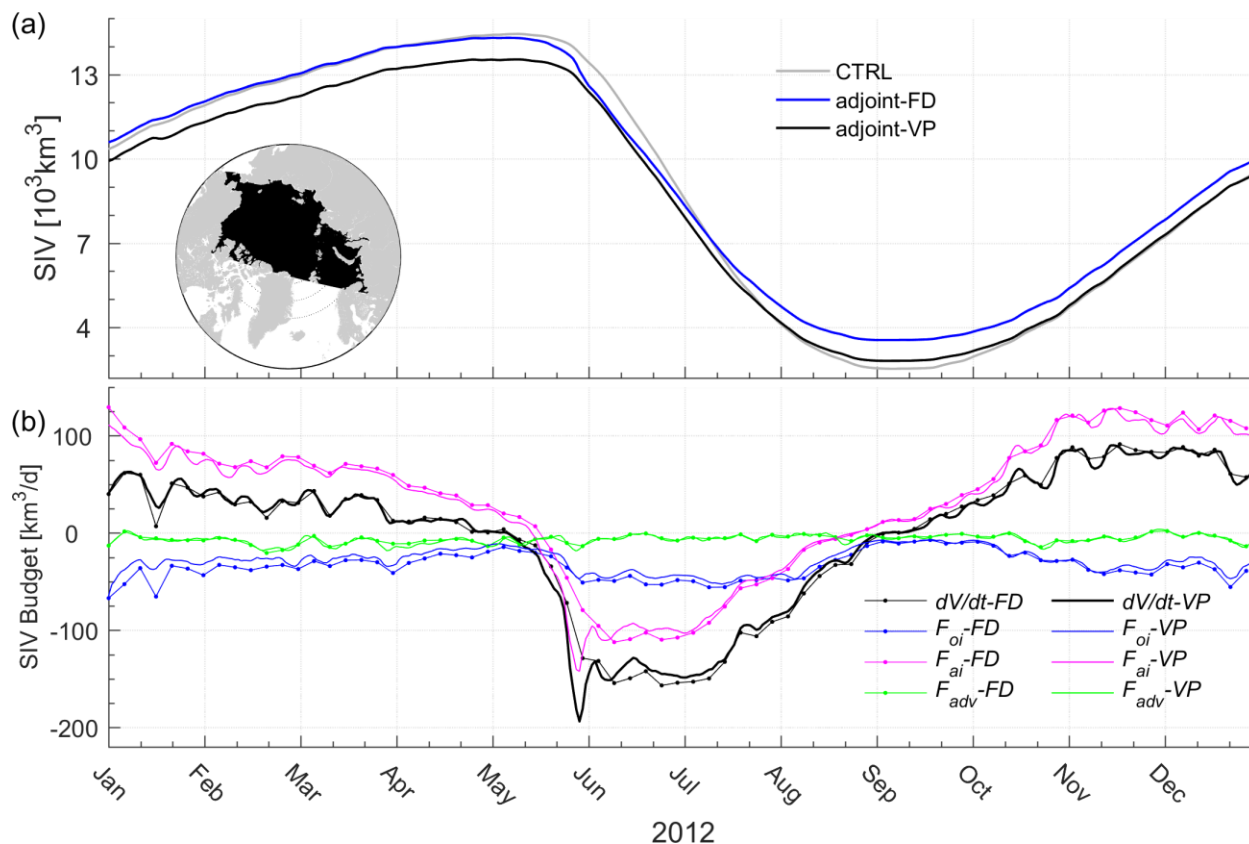
402 The mean SIT tendency  $\frac{dh}{dt}$  is dominated by the sea ice advective flux ( $-\nabla \cdot (\vec{u}h)$ ), ocean-sea ice heat flux ( $F_{oi}$ )  
 403 at the sea ice bottom, atmosphere-sea ice flux ( $F_{ai}$ ) at the sea ice surface, and a residual term ( $F_{res}$ ) including a snow  
 404 flooding effect and a source term to correct negative mean SIT to zero.  $F_{oi}$  depends on ocean temperature difference  
 405 from freezing temperature (Maykut and Mcphee, 1995) and  $F_{ai}$  consists of the radiation and turbulence fluxes over  
 406 the sea ice surface. The contributions of the residual terms are small and therefore we do not show them in the analysis  
 407 below.

408 Integrate the mean SIT over the Arctic Ocean (see Figure 9 for the locations), we derive Arctic sea ice volume  
 409 (SIV) changes. As shown in Figure 9a, the two assimilation runs change the total Arctic SIV changes in different ways.  
 410 Adjoint-VP reduces the Arctic SIV by reducing the initial Arctic SIV and changing the SIV tendency from May to  
 411 August. By September, adjoint-VP simulates more sea ice than the control run. Adjoint-FD slightly increases the  
 412 initial SIV, and the signals are invisible by February 2012. From May to July, adjoint-FD shows a stronger sea ice  
 413 melting process than the control run and adjoint-VP. By September, adjoint-FD simulates the most SIV among the  
 414 three simulations.

415 Based on Equation (10), we further compare SIV tendencies and the budget terms in the two assimilation runs  
 416 (Figure 9b). The two assimilation runs reveal that the seasonal SIV changes are dominated by  $F_{ai}$  (magenta lines in  
 417 Figure 9b). Throughout the year, the ocean melts the sea ice from the bottom (blue lines in Figure 9b) and net sea ice  
 418 transport also reduces the Arctic sea ice (green lines in Figure 9b). However, we note that a much stronger sea ice loss



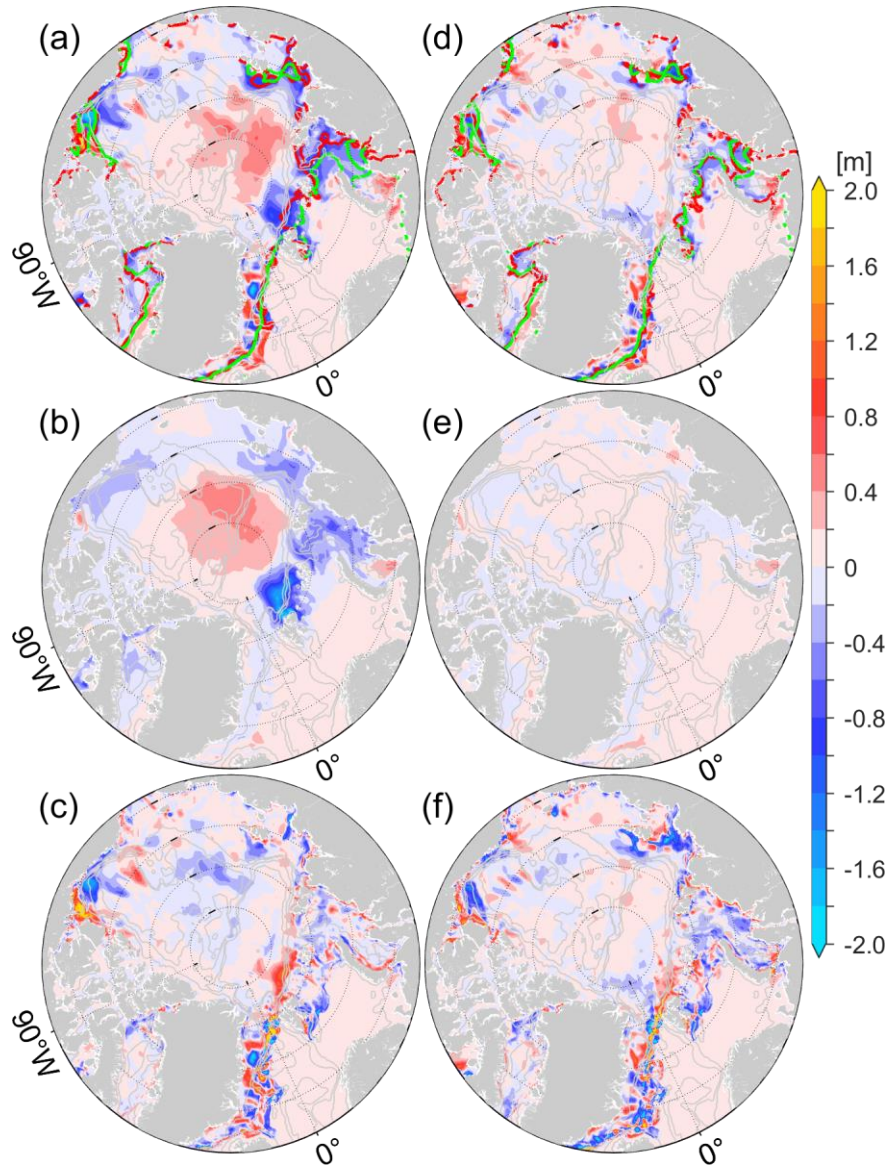
419 process occurs from May 20 to June 15 in adjoint-FD (up to  $-193.0 \text{ km}^3 \text{ day}^{-1}$ ) than in adjoint-VP (up to  $-125.0 \text{ km}^3$   
 420  $\text{day}^{-1}$ ), which is mainly attributed to  $F_{ai}$  anomalies (magenta lines in Figure 9b).  
 421



422  
 423  
 424 Figure 9. (a) SIV changes in the Arctic Ocean (see the bottom left subplot in Panel (a)) from January to December  
 425 2012. (b) SIV tendencies and contributions from  $F_{oi}$ ,  $F_{ai}$ , and  $F_{adv}$  in adjoint-FD and adjoint-VP (see the legend).  
 426

427 From May 20 to June 15, the Arctic Ocean observations rely most on satellite-measured SIC. Both the two  
 428 optimization runs reproduce the observed sea ice extents (SIEs, 15% SIC) well on June 15 (green and red lines in  
 429 Figure 10a, d), with adjoint-VP slightly better than adjoint-FD in the Barents and Kara Seas (Figure 10a, d).

430 On May 20, adjoint-FD simulates more sea ice than does adjoint-VP (Figure 9a). From May 20 to June 15,  
 431 adjoint-FD destroys the extra sea ice in the southeastern Beaufort Gyre, the Laptev Sea, the Kara Sea, and north of  
 432 Svalbard and Franz-Josef-Land through a stronger surface melting  $F_{ai}$  (Figure 10b). At the same time,  $F_{ai}$  results in  
 433 less sea ice loss (up to 0.6 m) in adjoint-FD in the central Arctic Ocean. Near the SIMs,  $F_{adv}$  differences determine the  
 434 mean SIT differences (Figure 10a, c). In contrast, mean SIT differences from May 20 to June 15 between adjoint-VP  
 435 and the control run (Figure 10d) are mostly caused by  $F_{adv}$  differences (Figure 10f) and  $F_{ai}$  differences have little  
 436 contribution (Figure 10e), indicating that adjoint-VP modifies the SID to improve the model simulation during this  
 437 period.

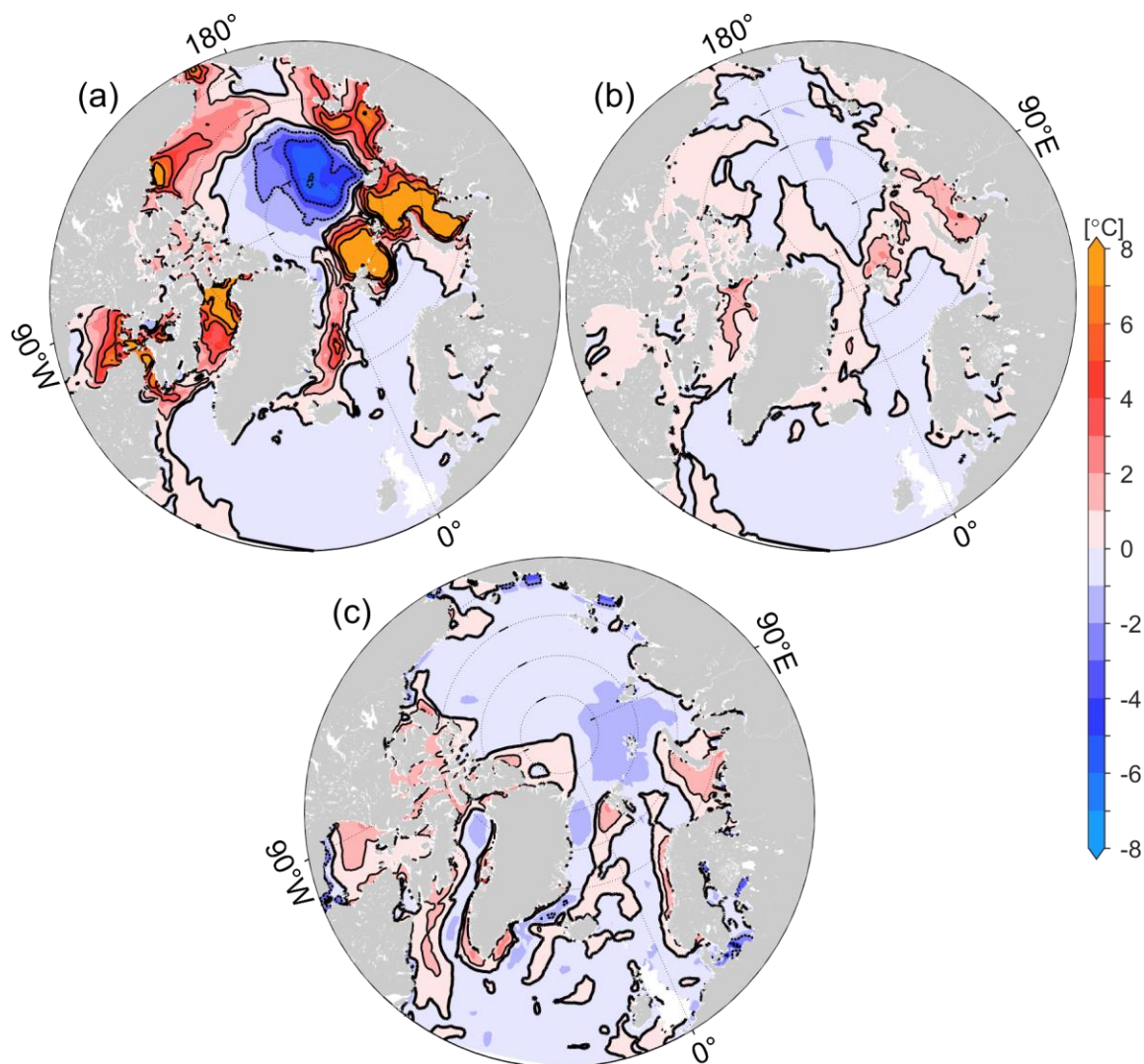


438

439 Figure 10. (a) Differences in  $\int \frac{dh}{dt}$  integrated from May 20 to June 15 between adjoint-FD and the control run (adjoint-  
 440 FD minus the control run), attributed to (b)  $\int F_{ai}$  and (c)  $\int F_{adv}$  differences. Panels (c)-(f) are the same as Panels (a)-  
 441 (c) but for adjoint-VP. The red and green lines in Panels (a) and (d) indicate the model-simulated (a for adjoint-FD; d  
 442 for adjoint-VP) and satellite-observed SIEs on June 15.  
 443

444 From May 20 to June 15, the significant sea surface melting anomalies (Figure 10b) are mainly caused by 2-m  
 445 air temperature adjustments in adjoint-FD (Figure 11a). As shown, the 2-m air temperature is increased by more than  
 446 8 °C in the marginal seas (prior air temperature uncertainties are ~2-5 °C) to facilitate the intense surface melting. In  
 447 the central Arctic Ocean, the 2-m air temperature is reduced by -6 °C (Figure 11a), resulting in less sea ice loss up to  
 448 0.6 m (Figure 10b) than in the control run. In contrast, adjoint-VP adjusts the 2-m air temperature within  $\pm 3$  °C in the  
 449 marginal seas (Figure 10b), and the adjustments have little impact on the sea ice surface melting anomalies (Figure  
 450 10e). The 2-m air temperature differences averaged from May 20 to June 15 between the ERA5 and NCEP-RA1  
 451 reanalyses are within  $\pm 3$  °C (Figure 11c), indicating that adjoint-FD over-adjusts the 2-m air temperature to destroy

452 the extra sea ice. Again, the spatial patterns 2-m air temperature adjustments in adjoint-FD and adjoint-VP don't  
453 resemble that of ERA5-NECP differences.  
454



455  
456 Figure 11. Adjustments of the 2-m air temperature averaged from May 20 to June 15, 2012, in (a) adjoint-FD and (b)  
457 adjoint-VP. Panel (c) shows the 2-m air temperature differences between the ERA5 and NCEP-RA1 reanalyses  
458 (ERA5 minus NCEP-RA1) averaged from May 20 to June 15, 2012.  
459

460 In summary, the two optimisation runs successfully reproduce the sea ice retreat process in 2012 by assimilating  
461 satellite and in situ measurements. However, the sea ice retreat processes differ in the two optimised simulations,  
462 especially from May to June, when Arctic Ocean observations rely mostly on satellite-measured SIC. Considering the  
463 amplitude of the 2-m air temperature adjustments, the adjustments of the control variables in adjoint-VP are more  
464 reasonable than those in adjoint-FD due to the inclusion of the approximate adjoint of sea ice rheology.

## 465 **6 Conclusions**

466 The adjoint model is a powerful way to calculate the sensitivities of a target function to model variables and has  
467 been applied to coupled Arctic ocean and sea ice models for sensitivity studies (Heimbach et al., 2010; Kauker et al.,  
468 2009; Koldunov et al., 2013) and state estimations (Fenty and Heimbach, 2013; Koldunov et al., 2017; Lyu et al.,  
469 2021b; Nguyen et al., 2021). However, due to the persistent instability issues, the adjoint of sea ice dynamics is  
470 traditionally excluded or simplified to the adjoint of a free-drift sea ice dynamic, which potentially hampers the  
471 accuracy of the coupled ocean and sea ice estimation.

472 Based on the study of Toyoda et al. (2019) and the coupled ocean and sea ice modelling and adjoint assimilation  
473 system (Lyu et al., 2021a), we approximate the adjoint of a viscous-plastic sea ice dynamic and test the impacts on  
474 estimating the spatiotemporal variations in the Arctic ocean and sea ice state.

475 Two optimisations are performed, one including and one excluding the adjoint of sea ice rheology. Both  
476 assimilation experiments reduce SIC and SIT errors and reproduce the sea ice retreat well. With the improved SIC  
477 retreat processes, adjoint-FD and adjoint-VP also show similar ocean temperature changes in the marginal seas and  
478 the southern Beaufort Gyre, as solar radiation heats the open water quickly as the sea ice retreats. With the improved  
479 adjoint of sea ice dynamics, adjoint-VP allows much stronger adjustments of the initial temperature, resulting in a  
480 more significant improvement on the temperature in the North Atlantic Ocean and the intermediate layer (50-700 m)  
481 of the Arctic Ocean.

482 Although that adjoint-FD computes much stronger sensitivities of the cost function to the wind vectors than does  
483 adjoint-VP, we note that adjoint-FD adjusts more (less) of the 2-m air temperature (wind vectors) than does adjoint-  
484 VP. It is evident that the adjoint sensitivities of wind vectors in adjoint-FD less efficiently reduce the cost function  
485 than those in adjoint-VP during the optimisation. Adjoint-FD strongly adjusts the 2-m air temperature to reduce the  
486 model-data misfits while adjoint-VP slightly adjusts all the control variables to improve the model simulation.

487 Using sea ice budget analysis, we further examine the sea ice retreat processes in adjoint-FD and adjoint-VP. We  
488 note that adjoint-FD and adjoint-VP show different sea ice thinning processes from May 20 to June 15 and in the  
489 marginal seas. Adjoint-FD destroys the extra sea ice in the marginal seas by substantially increasing the 2-m air  
490 temperature (up to 8 °C), which is much larger than the ERA5-NCEP differences. In adjoint-VP, the sea ice thinning  
491 is moderate with more reasonable adjustments of 2-m air temperature (within  $\pm 3$  °C) and the size of the adjustments  
492 are much smaller than the ERA5-NCEP differences. Therefore, by including the adjoint of sea ice rheology, adjoint-  
493 VP projects the model-data misfits more properly to the control variables than that in adjoint-FD.

494 Parameter uncertainties significantly impact ocean and sea ice simulations (Lu et al., 2021; Massonnet et al.,  
495 2014; Sumata et al., 2019), and a lack of direct observations of key parameters potentially results in biases in the  
496 model simulations and predictions. The development of the adjoint of the viscous-plastic sea ice dynamics further  
497 introduces three parameters, including the ice compressive strength constant ( $P^*$ ), ice strength decay constant ( $C^*$ ),

498 and ratio of normal stress to shear stress ( $e$ ), into the adjoint model. Since it remains unclear how well the tangent  
499 linear approximation could represent the relations between the model parameters and the model state, in the future  
500 studies, we will examine the accuracy of the adjoint sensitivities with respect to the model parameters and then further  
501 improve the ocean-sea ice estimations by jointly estimating the state and parameters.

## 502 **7 Data availability**

503 The data used to create the plots in the paper are available at Pangaea (<https://issues.pangaea.de/browse/PDI-33039>).  
504 Assimilated observations are listed in Table 1; and the up-looking sonar observed sea ice draft are from the Beaufort  
505 Gyre Exploration Project (BGEP, <https://www2.who.edu/site/beaufortgyre/>).

506  
507 *Author contribution.* G. Lyu designed the experiments, conducted the experiments and analysis. A. Koehl contributed  
508 to the experiment design and interpretations. G. Lyu wrote the first draft. A. Koehl, D. Stammer, X. Wu, and M. Zhou  
509 contributed to reviewing and editing the manuscript.

511 *Competing interests.* The authors declare that they have no conflict of interest.

512

## 513 **Acknowledgments**

514 This work was funded partly by the Open Fund Project of Key Laboratory of Marine Environmental Information  
515 Technology, Ministry of Natural Resources of the People's Republic of China to G. Lyu and by the Shanghai Frontiers  
516 Science Center of Polar Science (SCOPS) to M. Zhou. We thank NCEP and ECMWF for offering the NCEP/NCAR-  
517 RA1 and ERA5 reanalyses. Thanks to ICDC at University of Hamburg and Alfred Wegener Institute for supplying  
518 the ASI-SSM/I sea ice concentration and CryoSat-2/SMOS L4 datasets. We also acknowledge the Met Office, the  
519 Copernicus Marine Service, and the Beaufort Gyre Exploration Project for archiving and sharing the EN4, the along-  
520 track SLA, and sea ice draft datasets used in assimilation and independent validation.

521

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